

Fluctuation induced non-canonical BCS states: A mechanism for pseudogap

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Abstract. – We pose the question of what effect the statistical fluctuation causes if it induces a non-unitary evolution. We apply this idea to the BCS model and study fluctuation around the mean-field average. We find that, dynamics of the thermalization influences the equilibrium besides the non-unitary evolution, and the resulting equilibrium state is no longer the canonical one. The pseudogap phenomenon can exist in this model.

Introduction. – Consider equilibrium states of a system governed by master equation

$$\frac{d\rho}{dt} = -i[\hat{H}, \rho] - \eta[\hat{A}, [\hat{A}, \rho]], \quad (1)$$

where \hat{A} is an operator of the system. The equation is a simplified Lindblad equation [1] with the operators specified as a Hermitian one. If an energy eigenstate $|E\rangle\langle E|$ is not an eigenstate of \hat{A} , it is in general not time-independent, $d(|E\rangle\langle E|)/dt \neq 0$. In this case, the canonical state $\rho \propto e^{-\hat{H}/k_B T}$ can not be an equilibrium state, and a non-canonical one is required. Suppose the goal of thermal relaxation is the canonical equilibrium ensemble¹. The thermalization ceases when the goal is achieved. When the system is in a non-canonical equilibrium state, however, the thermalization still works. So the dynamics of thermalization is also a factor in determination of the equilibrium.

The BCS theory is a non-interaction quasiparticle model. The subadditivity [2] of entropy for a composite system ρ^{AB} indicates $S(\rho^{AB}) \leq S(\text{Tr}_A[\rho^{AB}] \otimes \text{Tr}_B[\rho^{AB}])$. When there is no interaction between the two subsystems, this inequality can be generalized to the free energy as $F(\rho^{AB}) \geq F(\text{Tr}_A[\rho^{AB}] \otimes \text{Tr}_B[\rho^{AB}])$. As long as \hat{A} does not mix states of different momentum, according to the principle of minimum free energy, a BCS state after thermal relaxation must take the form $\rho = \otimes_{\mathbf{k}} \rho_{\mathbf{k}}$ [3], where

$\rho_{\mathbf{k}}$ is a density matrix in the subspace of momentum \mathbf{k} . So we can handle each subspace separately, which allow us to study the energy variation caused by a gap for each momentum. We assume that a gap emerges only in the subspaces where the energy is reduced by the gapping. For the gapped momentums, we adopt the Cooper approximation, a constant $\Delta_{\mathbf{k}}$.

Here, a subspace of momentum \mathbf{k} means the one spanned by the ground state component, two excitons and the double exciton:

$$\begin{aligned} |0\rangle &= |\Phi_{\mathbf{k}}\rangle = u_{\mathbf{k}} | \rangle + v_{\mathbf{k}} c_{\mathbf{k}\uparrow}^+ c_{-\mathbf{k}\downarrow}^+ | \rangle, \\ |1\rangle &= b_{-\mathbf{k}\downarrow}^+ |\Phi_{\mathbf{k}}\rangle = c_{-\mathbf{k}\downarrow}^+ | \rangle, \quad |2\rangle = b_{\mathbf{k}\uparrow}^+ |\Phi_{\mathbf{k}}\rangle = c_{\mathbf{k}\uparrow}^+ | \rangle, \\ |3\rangle &= b_{\mathbf{k}\uparrow}^+ b_{-\mathbf{k}\downarrow}^+ |\Phi_{\mathbf{k}}\rangle = -v_{\mathbf{k}}^* | \rangle + u_{\mathbf{k}}^* c_{\mathbf{k}\uparrow}^+ c_{-\mathbf{k}\downarrow}^+ | \rangle, \end{aligned} \quad (2)$$

where $| \rangle$ is the bare vacuum, $b_{\mathbf{k}\uparrow}^+, b_{-\mathbf{k}\downarrow}^+$ the Bogoliubov creation operators and $c_{-\mathbf{k}\downarrow}^+, c_{\mathbf{k}\uparrow}^+$ creation operators of an electron. The subspace spanned by states of $\mathbf{k}\downarrow$ and $-\mathbf{k}\uparrow$ are referred to by $-\mathbf{k}$.

To have a sense of how we can deal with a subspace separately, let us derive the Fermi-Dirac distribution for the BCS model according to the principle of minimum free energy. A density operator in a subspace can be expressed as $\rho_{\mathbf{k}} = \sum_{mn} a_{mn} |m\rangle\langle n|$ with $a_{mn}^* = a_{nm}$. Since the time-independent states of von Neumann equation are energy eigenstates, an equilibrium state has form $\rho_{\mathbf{k}} = \sum_{n=0}^3 a_{nn} |n\rangle\langle n|$. We assign variables as $a_{00} = p_-, a_{33} = p_+, a_{11} = a_{22} = (1 - p_- - p_+)/2$ and set the energy of the ground states zero. Then we have

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¹The argument is given in the Appendix.

$E^1 = E^2 = E^3/2 = E_{\mathbf{k}} = \sqrt{\omega^2 + \Delta^2}$, $\omega = \epsilon_{\mathbf{k}} - \epsilon_F$. By minimizing the free energy, we obtain the probabilities

$$p_{\mp} = (e^{\mp\beta E_{\mathbf{k}}} + 1)^{-2}, \quad (3)$$

where $\beta = k_B T$. The Fermi-Dirac distribution is given by $(1 - p_- + p_+)/2 = (e^{\beta E_{\mathbf{k}}} + 1)^{-1}$

Non-unitary evolution and thermalization. – A many-body Hamiltonian can not lead to non-unitary evolution by itself, because no environment is involved. For a part of this many-particle system, however, the other parts actually play a roll as an environment with fluctuations, which can cause decoherence [4]. Consider the subspace of momentum \mathbf{k} , Hamiltonian for which is given by

$$H_{\mathbf{k}} = E_{\mathbf{k}}(b_{\mathbf{k}\uparrow}^+ b_{\mathbf{k}\uparrow} + b_{-\mathbf{k}\downarrow}^+ b_{-\mathbf{k}\downarrow}) + P, \quad (4)$$

where P is the fluctuation around the mean field average

$$P = c_{\mathbf{k}\uparrow}^+ c_{-\mathbf{k}\downarrow}^+ (-g) \sum_{\mathbf{k}'} (c_{-\mathbf{k}'\downarrow} c_{\mathbf{k}'\uparrow} - \langle c_{-\mathbf{k}'\downarrow} c_{\mathbf{k}'\uparrow} \rangle) + c.c. \quad (5)$$

From $c_{-\mathbf{k}\downarrow} c_{\mathbf{k}\uparrow} = (\Delta_{\mathbf{k}}/E_{\mathbf{k}})(1 - n_{-\mathbf{k}\downarrow} - n_{\mathbf{k}\uparrow})$, P is actually a fluctuation concerning the particle number in gapped states, and it sets off when a gap emerges. To have an explicit expression of the non-unitary dynamics cause by this fluctuation, we assume the fluctuation can be approximated by a Gaussian noise. The trivial equality $\langle c_{-\mathbf{k}'\downarrow} c_{\mathbf{k}'\uparrow} \rangle - \langle c_{-\mathbf{k}'\downarrow} c_{\mathbf{k}'\uparrow} \rangle = 0$ indicates that the fluctuation is a non-biased noise. We specify the phase factor so that $\Delta_{\mathbf{k}}$ is a real number. Then the subspace is coupled to the noise though operator $\hat{A} = c_{\mathbf{k}\uparrow}^+ c_{-\mathbf{k}\downarrow}^+ + c_{-\mathbf{k}\downarrow} c_{\mathbf{k}\uparrow}$ with coupling $-g$. In the “interaction picture” the non-unitary evolution has a Lindblad form [5]

$$\frac{d\rho_{\mathbf{k}}^I}{dt} = -g^2 \tau_c [\hat{A}, [\hat{A}, \rho_{\mathbf{k}}^I]] \quad (6)$$

where $\tau_c \equiv \int_0^\infty f(t)f(0)dt$ is the autocorrelation for $t = 0$, at which the gap is opened up. In the Schrödinger picture, Eq. (6) takes the form of Eq. (1).

Since eigenstates of \hat{A} are different from the energy eigenstates, we need to construct a thermalization model. Effect of the thermalization is reduction of the free energy. To achieve the canonical ensemble, we may expect a phenomenological description of the thermalization as the following: for off-diagonal elements a_{mn} , $m \neq n$, the time-dependence obeys

$$\frac{da_{mn}}{dt} = -f_{mn}(\rho_{\mathbf{k}})a_{mn}, \quad (7)$$

while diagonal elements a_{nn} vary with time as

$$\frac{da_{nn}}{dt} = -h_{nn}(\rho_{\mathbf{k}}) \frac{\partial F}{\partial a_{nn}}. \quad (8)$$

Here, $f_{mn}(\rho_{\mathbf{k}})$, $h_{nn}(\rho_{\mathbf{k}})$ are positive functions of $\rho_{\mathbf{k}}$ representing thermalization properties of the system, and

$$F = a_{nn} E^n + T k_B a_{nn} \ln a_{nn} \quad (9)$$

is the free energy without considering the off diagonal elements. For simplicity, we consider the functions two constants, $2f$ and $2h$ respectively. The factor 2 is included to simplify latter notation.

The overall dynamics of our BCS model consists of three components, that is, the von Neumann equation, the non-unitary evolution and the thermal relaxation (R), i.e.

$$\frac{d\rho_{\mathbf{k}}}{dt} = -i[\hat{H}, \rho_{\mathbf{k}}] - g^2 \tau_c [\hat{A}, [\hat{A}, \rho_{\mathbf{k}}]] + R \quad (10)$$

Without the non-unitary evolution, the off-diagonal elements vary as

$$a_{mn}(t) = a_{mn}(t_0) e^{i(E^n - E^m)t - ft} \quad (11)$$

which implies that they approach zero through relaxation. Then the von Neumann term gives zero because energy eigenstates are commutable with the Hamiltonian. The master equation (10) reduces to Eq. (8), where the time-independence is just the condition for minimum free energy. The solution is the canonical equilibrium state.

The pseudogap. – The operator $\hat{A} = c_{\mathbf{k}\uparrow}^+ c_{-\mathbf{k}\downarrow}^+ + c_{-\mathbf{k}\downarrow} c_{\mathbf{k}\uparrow}$ acts as:

$$\begin{aligned} \hat{A} | \rangle &= c_{\mathbf{k}\uparrow}^+ c_{-\mathbf{k}\downarrow}^+ | \rangle, \quad \hat{A} c_{\mathbf{k}\uparrow}^+ c_{-\mathbf{k}\downarrow}^+ | \rangle = | \rangle, \\ \hat{A} c_{-\mathbf{k}\downarrow} c_{\mathbf{k}\uparrow} | \rangle &= \hat{A} c_{\mathbf{k}\uparrow}^+ | \rangle = 0. \end{aligned} \quad (12)$$

Action of $[\hat{A}, [\hat{A}, \rho]]$ annihilate the state elements except $|m\rangle\langle n|$ ($m, n = 0, 3$). The non-unitary evolution impose no constraints on matrix elements a_{mn} ($m, n \neq 0, 3$). Those elements approach zero through thermal relaxation except a_{11} and a_{22} . We only need to consider the following matrix

$$\rho_{\mathbf{k}} = \begin{pmatrix} a_{00} & 0 & 0 & a_{03} \\ 0 & a_{11} & 0 & 0 \\ 0 & 0 & a_{22} & 0 \\ a_{30} & 0 & 0 & a_{33} \end{pmatrix}, \quad (13)$$

and solve the equations given by coefficients of the six state elements. Among the six equations, the two from $|1\rangle\langle 1|, |2\rangle\langle 2|$ have the same solution, and the two from $|0\rangle\langle 3|, |3\rangle\langle 0|$ are equivalent because of the Hermitian symmetry. So only four equations are independent.

It is more convenient to obtain the equilibrium state through equations from the coefficients of $| \rangle\langle |, c_{\mathbf{k}\uparrow}^+ c_{-\mathbf{k}\downarrow}^+ | \rangle\langle |, c_{-\mathbf{k}\downarrow} c_{\mathbf{k}\uparrow} | \rangle\langle |, c_{-\mathbf{k}\downarrow} c_{\mathbf{k}\uparrow}$ and $c_{-\mathbf{k}\downarrow}^+ | \rangle\langle |, c_{-\mathbf{k}\downarrow}$, which are given by

$$\begin{aligned} i u_{\mathbf{k}} v_{\mathbf{k}} (a_{00} - a_{33}) - (h + 2\eta) u_{\mathbf{k}} v_{\mathbf{k}} (a_{03} + a_{30}) + \\ \eta (u_{\mathbf{k}}^2 - v_{\mathbf{k}}^2) (a_{00} - a_{33}) + u_{\mathbf{k}}^2 \frac{\partial F}{\partial a_{00}} + v_{\mathbf{k}}^2 \frac{\partial F}{\partial a_{33}} = 0, \end{aligned} \quad (14)$$

$$\begin{aligned} -i u_{\mathbf{k}} v_{\mathbf{k}} (a_{00} - a_{33}) + (h + 2\eta) u_{\mathbf{k}} v_{\mathbf{k}} (a_{03} + a_{30}) - \\ \eta (u_{\mathbf{k}}^2 - v_{\mathbf{k}}^2) (a_{00} - a_{33}) + v_{\mathbf{k}}^2 \frac{\partial F}{\partial a_{00}} + u_{\mathbf{k}}^2 \frac{\partial F}{\partial a_{33}} = 0, \end{aligned} \quad (15)$$

$$\begin{aligned} -i E u_{\mathbf{k}}^2 a_{03} - i E v_{\mathbf{k}}^2 a_{30} + \eta (a_{03} - a_{30}) + \\ u_{\mathbf{k}} v_{\mathbf{k}} \left(\frac{\partial F}{\partial a_{00}} - \frac{\partial F}{\partial a_{33}} \right) = 0, \end{aligned} \quad (16)$$

$$\frac{\partial F}{\partial a_{11}} = 0, \quad (17)$$

where $\eta = g^2 \tau_c$.

From summation of Eq. (14) and Eq. (15), we have

$$\frac{\partial F}{\partial a_{00}} + \frac{\partial F}{\partial a_{33}} = 0. \quad (18)$$

Thus Eq. (17) holds according to $a_{11} = (1 - a_{00} - a_{33})/2$ and the chain rule of derivative. Owing to $\langle n_{\mathbf{k}\uparrow} \rangle + \langle n_{-\mathbf{k}\downarrow} \rangle = 1/2 - (a_{00} - a_{33})/2$, what concerns our discussion is the value of $a_{00} - a_{33}$. Eq. (18) gives relation

$$1 + (a_{00} - a_{33})^2 - 2(a_{00} + a_{33}) = 0. \quad (19)$$

Substituting it in $\partial F/\partial a_{00}$, we have

$$\frac{\partial F}{\partial a_{00}} = -E_{\mathbf{k}} + T k_B \ln \frac{1 + a_{00} - a_{33}}{1 - (a_{00} - a_{33})} \quad (20)$$

We see that Eq. (14) is a transcendental equation of $a_{00} - a_{33}$. To obtain an approximate solution, we consider the first order expansion of $a_{00} - a_{33}$ with limit of strong interaction, a large η , which leads to an approximate solution

$$a_{00} - a_{33} \simeq E_{\mathbf{k}} \left(\frac{\eta f \omega^2}{\hbar f E_{\mathbf{k}}^2 + 2\eta \hbar \Delta^2} + 2k_B T \right)^{-1}. \quad (21)$$

Our approximation requires $a_{00} - a_{33} \ll 1$. From the solution, this condition is ensured when Δ is a small number, $\Delta \sim 0$. When $\omega \sim 0$, a small $E_{\mathbf{k}} \sim 0$ makes $a_{00} - a_{33}$ a small number. For $\omega \sim 0$, a large η results in a small $a_{00} - a_{33}$. It is necessary to note that the solution not only applies to the gapped momentum, but also to the states ungapped. This is because the non-unitary evolution affects on all momentums as long as some momentums are gapped. For the gapped momentums, Δ equals the gap constant, while $\Delta = 0$ for those ungapped momentums.

According to our assumption, the gapping occurs only in the subspace where a gap reduces the energy. For an infinitesimal gap, the gapped momentum should satisfy $\left. \frac{d(\delta E_{\mathbf{k}})}{d(\Delta^2)} \right|_{\Delta^2=0} < 0$. With our approximation, the derivative is given by

$$\left. \frac{d(\delta E_{\mathbf{k}})}{d(\Delta^2)} \right|_{\Delta^2=0} \simeq \frac{1}{2\omega} - \frac{2\hbar}{f}. \quad (22)$$

For momentums near the Fermi surface, we have $\omega \sim 0$, so the gap for them can not be opened. With proper parameters f and \hbar , momentums having a distance to the Fermi surface can be gapped. Because the ungapped states can be excited without overcoming an energy gap, the overall state is not in the superconducting phase. Thus the pseudogap phenomenon emerges.

Conclusion. — We studied the non-unitary evolution caused by the fluctuation around the mean field average. We showed that such an evolution can break the superconducting gap for momentums near the Fermi surface and lead to the pseudogap phenomenon. Because the equilibrium state is a non-canonical one, dynamics of the thermal

relaxation also influence its form. In the non-canonical equilibrium states, the particle number does not obey the Fermi-Dirac distribution even in non-interaction Fermion systems.

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Appendix: Goal of thermalization. — Suppose an equilibrium ensemble of an N dimensional system is constituted by $|n\rangle = c_{nm}|E_m\rangle$, where $|E_m\rangle$ ($m = 1, 2, \dots, N$) is energy eigenstates. According to the principle of minimum free energy, the equilibrium state is given by

$$\rho = \frac{\exp(-\beta \sum_m |c_{nm}|^2 E_m) |n\rangle \langle n|}{\text{Tr}[\exp(-\beta \sum_m |c_{nm}|^2 E_m) |n\rangle \langle n|]} \quad (23)$$

Then, taking the partial derivatives with respect to c_{nm} , one can find the canonical equilibrium state ($a_{nm} = \delta_{nm}$) is a local minimum of the free energy, while other states are not in general. Of course, there may be other local minimums for delicate assignment of the parameters, and a rigid argument should show the canonical ensemble is the global minimum. In view of the common validity of the canonical ensemble, however, we assume it is the goal of thermal relaxation.